Nano Particle Physics

Nano Scale Systems. (01)

Unit - 1

1) What do you mean by Nano science and Nanotechnology?

→ (The term 'Nano' is derived from the Greek word 'nanos', which means 'dwarf'.) Nano refers to 10^{-9} that is one billionth part of something. Thus one nanometer (1 nm) means one billionth of a meter that is 10^{-9} m. One nanometer is on the scale of atomic diameter. Hydrogen atom diameter is about 0.1 nm.

(Nanoscience is study of structures and materials on the scale of nanometers. For using Nano science, at least one dimension of the material or structure should lie in the range of 1 to 100 nm. Nanoscience is the study of phenomena and manipulation of materials at atomics molecular and macromolecular scales.)

(Nanomaterials are defined as those materials which have structured components with size less than 100 nm is in at least one dimension.) When structures are made in small enough (that is in nanometer range), they aquire interesting and useful properties. In nano-regime properties of nanomaterials are quite different as compared to their bulk counterparts.

Some of the changes that may occure in the properties of materials for transformation from bulk to nano are as follows :—

- Solids can become liquids at room temperature, e.g. gold.
- Insulators can become conductors, eg. silicon.
- Inert materials can become catalyst, e.g. platinum.
- Stable materials can become combustible, e.g. aluminium.
- Opaque substances can become transparent eg. copper.

(Nanotechnology is the ~~tech~~ technology of designing and making functional objects at the nanoscale and the science underlying it called nanoscience.) Nanotechnology as defined by National Nanotechnology Initiative (NNI) of US, is the manipulation of matter with at least one dimension lying in the range of 1 to 100 nanometers. (In other words, nanotechnology is the design, characterization production and application of structures, devices and system on nanoscale.)

(Nanotechnology deals with both natural and artificial structures on the nanometer scale. This is a technology which is capable of manipulating even single atoms and molecules.) various field of science such as surface science, organic chemistry, molecular biology, semiconductor physics microfabrication,

molecular engineering etc. come under the umbrella of nanotechnology are nanoscale technologies.

2) What are Low Dimensional structures and Bulk Materials ?

→ When one or more dimensions of a material are continuously reduced from a macroscopic size and reach to a very small size of less than 100 nm, then its physical and chemical properties show dramatic changes from those of the bulk. With reduction in size, novel electrical, electronic, chemical, mechanical, magnetic and optical properties can be introduced in the material. The resulting structure is known as low-dimensional structure or low-dimensional system.

Low dimensional materials (nano materials) are those systems in which the wavefunctions of the electron is confined, at least in one of the three dimensions.

Bulk Material :- It is a three dimensional structure in which there is no confinement along any direction. All of its dimensions are larger than the exciton Bohr radius. The particle is free to move through out the volume of the material. No quantization of particle motion occurs that is particle have a continuous range of energies between a minimum and maximum.

The low dimension materials classified into

3. structures on the basis of dimensionality. These are — Quantum Well, Quantum Wire and Quantum Dot.

3. Define Quantum Well, Quantum Wire and Quantum Dot.

→ Quantum Well :- It is a two-Dimensional nanostructure in which there is confinement along one ~~dimensional~~ direction and particle is free to move in other two directions (i.e. in a plane). Particle posses discrete (or quantized) energies associated with the confinement dimension. Particle energies are continuous along the other two (unconfined) dimensions.

Quantum Wire :- It is a one dimensional nanostructure in which there is confinement along two directions and particle is free to move in the third direction. Particle has discrete energies associated with these two directions of confinement and continuous along the third (unconfined) direction.

Quantum Dot :- The extreme case in which confinement of the particle occurs in all the three directions, results in a zero-dimensional nanostructure, called quantum dot. In this

case, the number of degrees of freedom of the particle is zero. Particle has discrete energies associated with its motion along all the three directions. Example of zero dimensional objects are nano-particles, clusters, colloids, nanocrystals and fullerenes. Quantum dots are composed of several to a few thousand atoms.

4) How Quantum size effect characterize the properties of Nano materials ?

→ // Quantum Size effect :- The quantum size effect is a phenomenon observed in nanomaterials where their electronic, optical and magnetic properties deviate from those of the bulk material when the size of the material is reduced to the nanoscale. This effect ~~as~~ arises due to the confinement of electrons and holes within the nanomaterial, leading to changes in the energy levels and band structure.

The quantum size effects manifests it self in various properties of nanomaterials, leading to unique behaviors :-

Optical Properties :- Nanomaterials often exhibit size-dependent optical properties due to the quantum size effects. As the size of the material decreases, the bandgap increases, leading to a blue shift in the absorption and emission spectra. This effect is

particularly pronounced in quantum dots, which display tunable optical properties based on their size.

Electronic Properties:- The quantum size effect influences the electronic properties of nanomaterials by modifying their band structure and density of states. In metal nanoparticles, the confinement of electrons leads to the formation of discrete energy levels, resulting in unique electronic transport properties. In semiconductor nanomaterials, the increased band gap can lead to enhanced charge carrier mobility and reduced electron-hole recombination.

Magnetic Properties:- The quantum size effect also impacts the magnetic properties of nanomaterials. In magnetic nanoparticles, the confinement of electrons can lead to the formation of single-domain states, resulting in superparamagnetic behaviour. This effect is exploited in various applications, such as magnetic data storage, magnetic resonance imaging and drug delivery.

Thermal Properties:- The quantum size effect can significantly influence the thermal properties of nanomaterials. The thermal conductivity of nanomaterials can differ greatly from their bulk counterparts due to changes in the phonon dispersion relations and increased phonon scattering

at the nanoscale. This effect can be exploited to develop nanomaterials with enhanced thermoelectric properties, which have applications in energy ~~harvesting~~ harvesting and thermal management.

5) What is the reason or principle behind Quantum size effect?

→ The Quantum size Effect arises due to the ~~confinement~~ confinement of electrons within nanomaterials. When the size of these materials becomes comparable to the De-Broglie wavelength of electrons, it restricts the electrons motion, leading to discrete energy levels. This quantization of energy levels is the hallmark of Quantum size effect, profoundly affecting the materials physical and chemical properties.

6) What do you mean by Quantum confinement? Write down the consequences of Quantum confinement.

→ (In small nanocrystals (i.e. nanomaterials), the electronic energy levels are not continuous as in the bulk but are discrete because of the confinement of the electronic wave function to the physical dimensions of the particles. This phenomena is called quantum confinement.)

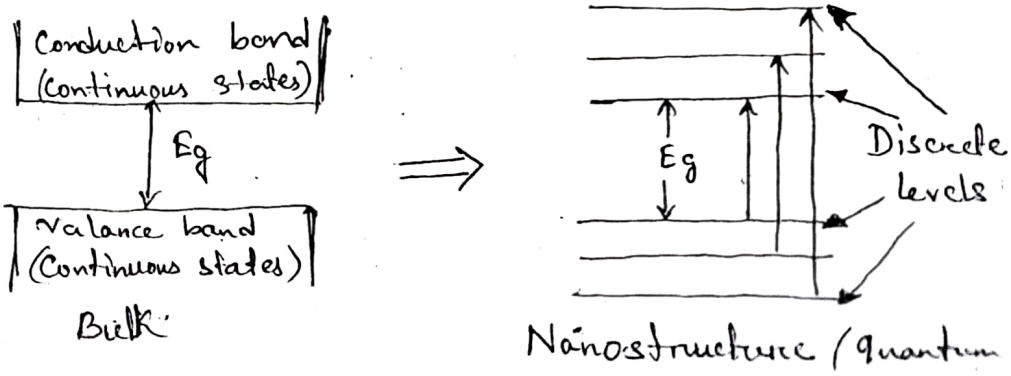


Figure:- Transition from continuous to discrete energy levels.

For a semiconductor particle, quantum confinement occurs when the nanocrystal radius becomes comparable to the ~~exiton~~ exciton Bohr radius. The confinement leads to a transition from continuous to discrete energy levels. When materials are so small that they lie in the quantum ~~regime~~ confinement regime, then their electronic and optical properties, deviate substantially from those of bulk materials are changed. The discrete structure of energy states leads to a discrete absorption spectrum for nanostructures.

A quantum confined structure is one in which the motion of electrons and holes are confined in one or more dimensions by potential barriers. If the charge carriers are confined in one direction and delocalized in other two directions, then the resultant structure is a quantum well. When the confinement occurs in two directions and the ~~delocalized~~ carriers are delocalized in the remaining third direction, then the resultant structure is a quantum wire or nanowire. A quantum dot exhibits confinement in all the ~~the~~ three dimensions. There is ~~to~~ no delocalization in this case. The following table summarizes

discrete.

The confinement and delocalization dimensions for various nanostructures —

Quantum Structure	Confinement Dimensions	Delocalization Dimensions
Bulk Conductor	0	3 (x, y, z)
Quantum well/Superlattices	1 (z)	2 (x, y)
Quantum wire	2 (x, y)	1 (z)
Quantum Dot	3 (x, y, z)	0

As more number of dimensions is confined, more discrete energy levels can be found, that is, carrier movement is strongly confined in a given dimension.

Nanostructure		Representation
Quantum Well	⟷	Particle in 1D box
Quantum Wire	⟷	Particle in 2D box
Quantum Dot	⟷	Particle in 3D box

The density of states D(E) determines the various electronic and other properties and differ dramatically for each of the three nanostructure type as shown in the below figure.

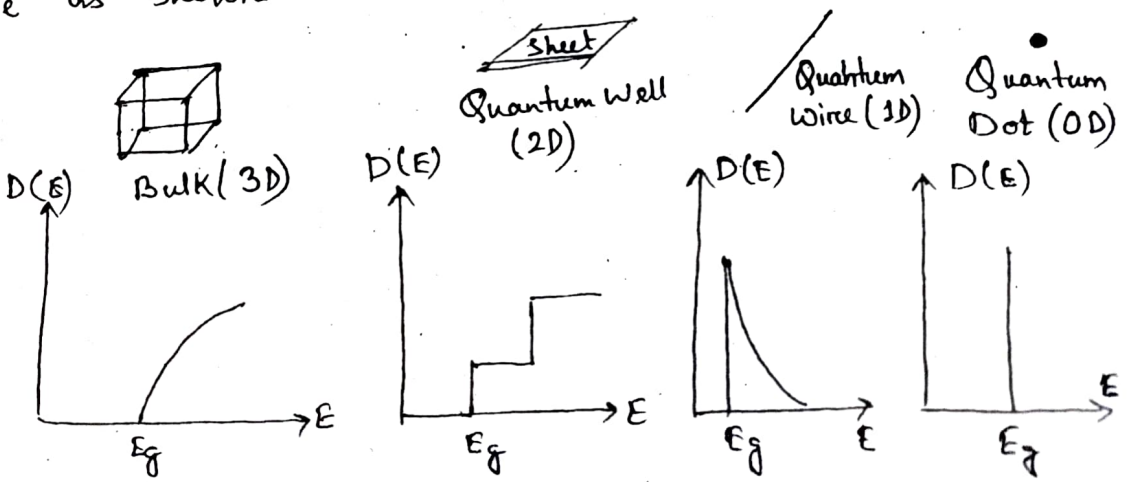


Fig:- Density of electron states for nanostructures.

Thus the nature of the dimensionality and of the confinement associated with a particular nanostructure have a noticeable effect on its properties.

7. Write down the examples of Quantum well, Quantum wire and Quantum Dots.

→ Quantum well :- Quantum wells are formed in semiconductors by having a material like gallium arsenide, sandwiched between two layers of a material with a wider bandgap like aluminum arsenide.

Quantum wire :- Carbon and silver nanotubes.

Quantum dots :- LEDs and solid state lighting, displays and photovoltaics.

8. Write the importance of defect in nanomaterials.

→ Defects in nanomaterials are crucial for tuning properties, enhancing reactivity and facilitating functionalities, thus enabling tailored properties and advancing various scientific and technological fields.

9. Write down some applications of nanoscale systems in various fields of science.

→ Nanomaterials in various scientific fields :-

Medicine and Healthcare :- Nanoparticles are being explored for drug delivery, targeting specific cells and tissues to improve treatement efficiency and reduce side effect. They are also used in imaging techniques for early disease detection.

Material Science :- Nanomaterials can be engineered to have unique properties like strength, conductivity and reactivity. This leads to lighter, stronger materials for construction and transportation and new catalysts for more efficient chemical reactions.

Electronics :- Nanoparticles are used in transistors, computer chips and other electronic devices to ~~miniaturi~~ miniaturize components and improve performance.

10. What do you mean by aspect ratio? How are the aspect ratio changed in nanomaterials when it is deviated from bulk? Explain with suitable example

→ Nanomaterials have a relatively greater surface area as compared to the same volume or mass of the same material in bulk form. The most important Quantum Size effect is the increase in surface to volume ratio for nanomaterials over bulk. This surface to volume ratio is defined as Aspect ratio for nanomaterials.

Surface area to volume ratio in nanoparticles have a

significant effect on the nanoparticles properties. Firstly, nanoparticles have a relative larger surface area when compared to the same volume of the material. for example, let us consider a sphere of radius r.

The surface area of the sphere will be = $4\pi r^2$

The volume of the sphere = $\frac{4}{3}\pi r^3$

Therefore, surface area to volume ratio will be

$$= \frac{4\pi r^2}{\frac{4}{3}\pi r^3} = \frac{3}{r}$$

It means that the surface area to volume ratio increases with the decrease in radius of the sphere and vice versa. It can also be conclude here that when given volume is divided into smaller piece, the surface area increases. Therefore as particle size decreases, a greater portion of the atoms are found at the surface compared to those inside. For example, a particle of size 3nm has 50% of its atoms on its surface, at 10 nm 20% of its atoms and at 30 nm has 5% of its atoms on its surface. Therefore nanoparticles have a much greater surface area per unit volume compared with the larger particles. (It leads to nanoparticles more chemically reactive. As chemical reaction occurs at surfaces, therefore a given mass of nanomaterial will be much more reactive than the same mass of material made up of large particles.) It is also found

that materials which are inert in their bulk form are reactive when produced in their nanoscale form.

11. ~~Show the densit~~ Derive an expression for density of states for bulk in three dimension.

→ In bulk (3D) material there is no confinement. Thus, there are three degrees of freedom and the electrons are free to move along all three (x, y, z) directions. The energy E is related to the propagation constant K as —

$$E = \frac{\hbar^2 K^2}{2m} \quad \text{, where } m \text{ is the mass of electron.} \qquad \text{—— (1)}$$

Consider the volume in reciprocal space (i.e. K space)

$$V_K = \frac{4}{3}\pi K^3 \qquad \text{where, } K^2 = K_x^2 + K_y^2 + K_z^2$$

$$\text{and } K_x = \frac{2\pi}{L_x} \; ; \; K_y = \frac{2\pi}{L_y}$$

$$K_z = \frac{2\pi}{L_z}$$

Here L_x, L_y, L_z are the length of the material along x, y, z directions. The factor of 2π occures due to the application of periodic boundary conditions on the materials. A set of (K_x, K_y, K_z) values represents a mode. Thus volume occupied by each mode is

$$= K_x \cdot K_y \cdot K_z = \frac{(2\pi)^3}{L_x \cdot L_y \cdot L_z}$$

Therefore the number of modes in ~~this~~ spec spherical volume V_K are given by —

$$= \frac{\text{volume of sphere}}{\text{volume of each mode}} = \frac{V_K}{K_x K_y K_z}$$

Mode – A mode is usually refers to a specific excitation or wave characterized by a particular wave vector K. For example, phonon modes are vibrational modes in a crystal characterised by a specific wave vector and frequency. In this case mode represents the wavevectors.

$$= \frac{\frac{4}{3}\pi K^3}{\frac{(2\pi)^3}{L_x \cdot L_y \cdot L_z}}$$

For electrons, there are two states (spin up and spin down) with same energy, then the number of electron states (or modes) in the volume V_k are -

$$= 2 \times \frac{\frac{4}{3}\pi K^3}{\frac{(2\pi)^3}{L_x L_y L_z}}$$

$$= \frac{K^3}{3\pi^2} L_x L_y L_z$$

The number of electron states per unit volume of the material, $N = \frac{\text{Total number of states}}{\text{Volume of the specimen}}$

$$= \frac{\frac{K^3}{3\pi^2} L_x L_y L_z}{L_x L_y L_z} = \frac{K^3}{3\pi^2} \quad \text{(iii)}$$

Density of states - $g(E) = \frac{dN}{dE} = \frac{d\left(\frac{K^3}{3\pi^2}\right)}{dE}$

$$= \frac{1}{3\pi^2} \cdot \frac{3K^2 dK}{dE} = \frac{K^2}{\pi^2}\left(\frac{dK}{dE}\right) \quad \text{(iv)}$$

From equation (i), $K^2 = \frac{2mE}{\hbar^2}$

or, $2K \cdot \frac{dK}{dE} = \frac{2m}{\hbar^2}$

or, $\frac{dK}{dE} = \sqrt{\frac{\hbar^2}{2mE}} \cdot \frac{m}{\hbar^2} = \sqrt{\frac{m}{2 \cdot \hbar^2 E}}$

∴ using these values in equation (iv);

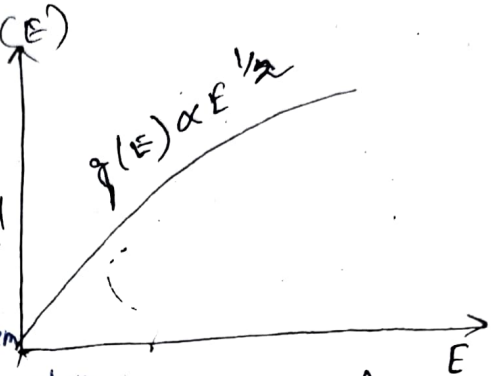
$$\therefore g(E) = \frac{2m E}{\pi^2 \hbar^2} \sqrt{\frac{m}{2\hbar^2 E}}$$

$$2 \times \frac{1}{2} \quad \frac{2}{2^{1/2}(\hbar^2)^{1/2}} \quad 2^{1-\frac{1}{2}} = \frac{1}{2}$$

$$\text{or, } g(E) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$$

This is the density of states in three dimensions.

So, $g(E) \propto E^{1/2}$



Thus ~~an~~ density of states of a bulk three dimensional material is a periodic function of its energy. Density of states in 3-D system increases with increase in energy of the system.

12. Derive an expression for Density of states of Quantum well in two dimension.

→ In two dimensional material such as a quantum well, electron motion is confined along one direction (say z) and they are free to move along other two directions (x, y). Thus electron energy is quantized along one ~~direction~~ dimension. The total energy along the quantized direction and the energy along the other two (i.e. free) directions It can be expressed as –

$$E = \frac{\hbar^2 K_z^2}{2m} + \frac{\hbar^2 k^2}{2m} = E_n + E_{x,y}$$

where $K^2 = K_x^2 + K_y^2$ and $K_z = \frac{n\pi}{L_z}$. Here $n = 1, 2, 3 \cdots$ is an interger.

Let, us consider the circular area of K space –

$$A_K = \pi K^2$$

Hence along x and y directions the particle is free to move, therefore due to periodic boundary conditions

$$K_x = \frac{2\pi}{L_x} \; ; \quad K_y = \frac{2\pi}{L_y} \; ;$$

Area of each mode $= K_x \cdot K_y = \frac{(2\pi)^2}{L_x L_y}$

Total number of modes in Area A_K is given by

$$= \frac{\text{Total area}}{\text{Area of each mode}} = \frac{\pi k^2}{\frac{(2\pi)^2}{L_x L_y}} = \frac{k^2}{4\pi} L_x L_y$$

If the particle be an electron, then there can be two electrons corresponding to same energy, one with spin up and the other with spin down. Therefore total number of energy states in the area πk^2 are given by

$$= 2 \cdot \frac{k^2}{4\pi} L_x L_y = \frac{k^2}{2\pi} L_x L_y \quad \text{——— (iv)}$$

Number of states per unit area —

$$N = \frac{\text{Total number of states}}{\text{Area}}$$

$$= \frac{\frac{k^2}{2\pi} L_x L_y}{L_x L_y} = \frac{k^2}{2\pi}$$

Density of states,

$$g(E) = \frac{dN}{dE} = \frac{d}{dE}\left(\frac{k^2}{2\pi}\right) = \frac{k}{\pi}\left(\frac{dk}{dE}\right)$$

Now, $E = \frac{\hbar^2 k^2}{2m} \Rightarrow k^2 = \frac{2mE}{\hbar^2}$

or, $2k\frac{dk}{dE} = \frac{2m}{\hbar^2}$ or, $k\frac{dk}{dE} = \frac{m}{\hbar^2}$ $\Rightarrow \sqrt{\frac{\hbar^2}{2mE}} \cdot \frac{m}{\hbar^2} = \sqrt{\frac{m}{2E\hbar^2}}$

So, $g(E) = \frac{m}{\pi\hbar^2}$ ——— (v)

This is the energy density of the ~~subband~~ subband for given K_z (or E_n). For each successive K_z there will

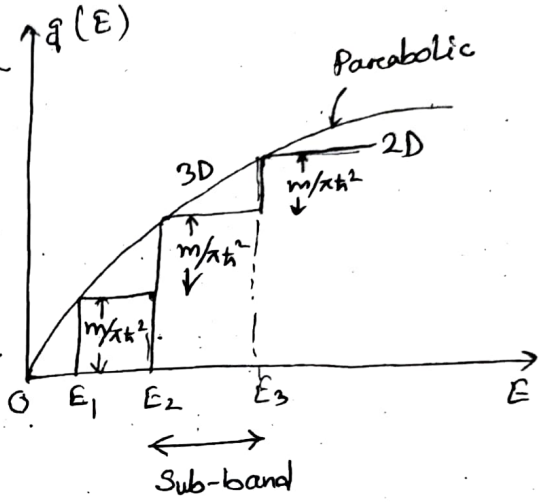
be an additional $\frac{m}{\pi\hbar^2}$ term and hence another subband. The density of states therefore expressed as –

$$g(E) = \frac{m}{\pi\hbar^2} \sum \theta(E - E_n) \quad \text{——— (vi)}$$

where θ is the Heaviside func or unit step func and is given by –

$$\theta(E - E_n) = \begin{cases} 0 & \text{for } E < E_n \\ 1 & \text{for } E > E_n \end{cases} \quad \text{— (vii)}$$

The plot of $g(E)$ versus E for a 2D material like quantum well is shown is figure (The resulting density of states for a quantum well is a staircase.)



Clearly in each subband, (the density of states is a constant that is independent of energy. The difference in the density of states of two consecutive sub-bands is $\frac{m}{\pi\hbar^2}$.)

13. Discuss about the density of states in one dimension of Quantum wire.

→ In a 1D material such as a quantum wire, particle motion is confined in two directions (y, z) and free along one dirⁿ (say x). Thus there is only one degree of freedom. Particle is quantized for motion along y and z dirⁿs. Thus energy Total energy of system can be written as sum of the energy along quantized directions (y, z) and the energy along the free dirⁿ(x) that is –

$$E = \frac{\hbar^2 K_y^2}{2m} + \frac{\hbar^2 K_z^2}{2m} + \frac{\hbar^2 K^2}{2m} = E_y + E_z + E_x \quad \text{——— (i)}$$

Where $K = K_x = \frac{2\pi}{L_x}$. For the confined dirns, we have

$$K_y = \frac{l\pi}{L_y} \; ; \quad K_z = \frac{n\pi}{L_z}$$

where $l, n = 1, 2, 3 \ldots$ are integers. We consider a length $2K$ in K space. The number of modes (states) along this length

$$= \frac{2K}{K_x} = \frac{2K}{2\pi/L_x} = \frac{K}{\pi} L_x$$

If the particle be an electron then there can be two electrons one with spin up and other with spin down corresponding to each energy. Therefore the number of states along the length K_x is —

$$= \frac{2K}{\pi} L_x$$

$\therefore$ No. of states per unit length $= N = \frac{\frac{2K}{\pi} L_x}{L_x} = \frac{2K}{\pi}$

Now, $K = \sqrt{\frac{2mE}{\hbar^2}}$

So, No. of states per unit length, $N = \frac{2}{\pi}\sqrt{\frac{2mE}{\hbar^2}}$

$\therefore$ Density of states is given by —

$$g(E) = \frac{dN}{dE} = \frac{2}{\pi}\sqrt{\frac{2m}{\hbar^2}}\frac{1}{2\sqrt{E}} = \frac{1}{\pi}\sqrt{\frac{2m}{\hbar^2 E}}$$

This is the energy density for a given n, l value or (E_n, E_l combination). This clearly shows that the density of states of a one dimensional system (quantum wire) decreases with increase in energy for every (n, l) combination.

By taking into account all n,l combinations the complete expression for density of states is expressed as

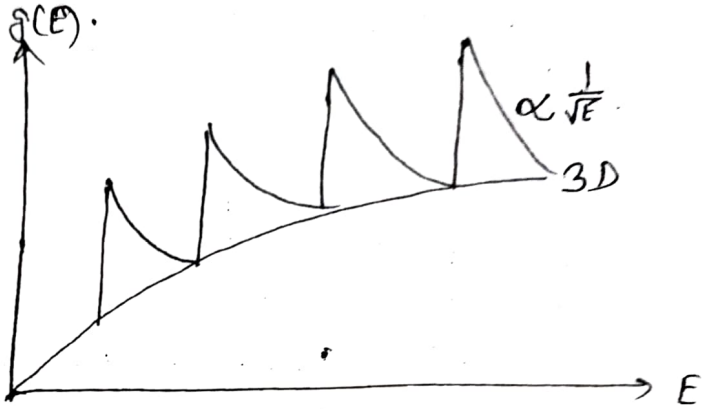
$$g(E) = \sqrt{\frac{2m}{\pi^2\hbar^2}} \sum_{n,l} \frac{1}{\sqrt{E-E_{n,l}}} \theta(E-E_{n,l})$$

where $\theta(E-E_{n,l})$ is the Heaviside or unit step function.

The plot of $g(E)$ versus E for a quantum wire is shown in the give figure.

The density of states of a 1-D system decreases with increase in energy for every (n,l) combination

$$g(E) \propto \frac{1}{\sqrt{E}}$$



14. Discuss about the density of states in Zero dimension of Quantum Dot.

→ In the extreme case of confinement along all the three directions, particle is not free to move at all. Its motion is confined along all the three directions x, y, z. The resultant material or nanostructure is called a quantum dot or nanoparticle. The energy of the particle is quantized along all the three directions x, y, z. Therefore total energy of the system is quantized and is given by -

$$E = \frac{\hbar^2 K_x^2}{2m} + \frac{\hbar^2 K_y^2}{2m} + \frac{\hbar^2 K_z^2}{2m} = E_l + E_n + E_p \quad \text{—(1)}$$

Where $l, n, p = 1, 2, 3 \ldots$ are integers.

Also, $K_x = \frac{l\pi}{L_x}$; $K_y = \frac{n\pi}{L_y}$; $K_z = \frac{p\pi}{L_z}$

In this case there is no K-space to be filled with electrons and all available states exist only at discrete energies. Hence the density of states for a zero dimensional (0D) system that is a quantum dot is expressed by a ~~dentu~~ delta func as —

$$g(E) = \delta(E - E_{n,l,p})$$

figure shows the plot of $g(E)$ versus E for a zero dimensional material.

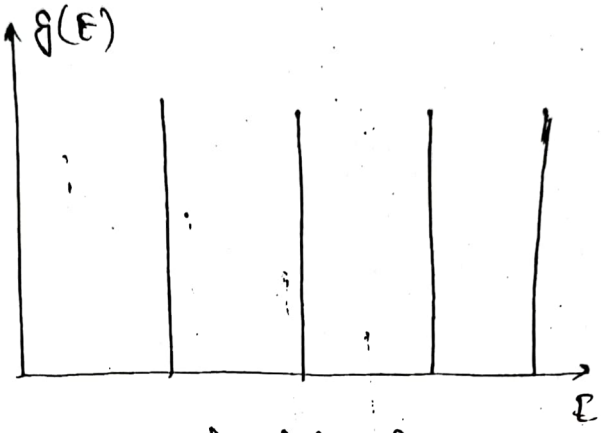


Fig: Density of states for ideal quantum dots.

In real quantum dots, the size distribution leads to a broadening of the delta (line) function as shown in the figure.

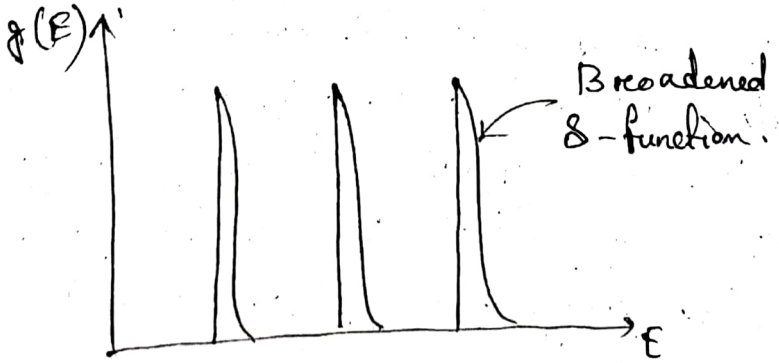


Fig: DOS for Real Quantum Dots.

15. Explain - a quantum dot can be a nanodot but the reverse is not necessarily true.

→ If length, breath and thickness of the quantum well lie in the nanorange, then the nanostructure that we have is essentially a nanodot. If this nanodot exhibits quantum properties, then it is called a quantum dot. Thus a quantum dot can also be a nanodot, but the reverse is not necessarily true.

16. What do you mean by Nanorods ? How do they differ from nanowires ?

→ Nanorods are type of nanostructure characterized by their elongated, rod-like shape with dimensions typically in the nanometer scale (1 - 100 nm in diameter and up to several micrometers in length). They possess unique optical, electronic and chemical properties due to their high aspect ratio and shape anisotropy. The synthesis methods for nanorods include chemical vapor deposition, solution-phase synthesis and template-based methods.

Nanowires, on the other hand, are similar to nanorods in their elongated structure but differ primarily in their higher aspect ratio and continuous crystalline structure. Nanowires typically have a uniform diameter and can extend to lengths of several micrometers or more. They are often used in electronic applications due to their superior electrical conductivity and ability to form continuous paths for electron transport.

The key differences between nanorods and nanowires are ;—

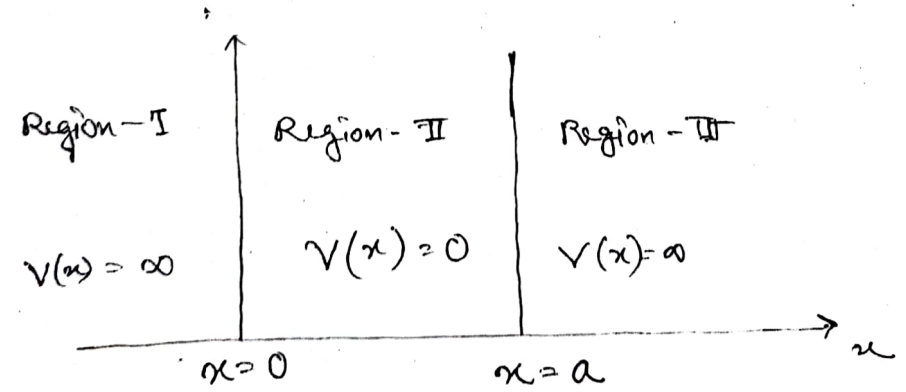
1. Aspect Ratio :- Nanorods have a lower aspect ratio compared to nanowires, which are significantly longer relative to their diameter.

2. Crystallinity :- Nanowires generally have a continuous crystalline structure, which is essential for application in nanoelectronics.

3. Applications :- Nanorods are commonly used in applications where tunable optical properties are required, such as in photonic devices and sensors. Nanowires are ~~favoured~~ used in electronic and energy applications due to their high electrical conductivity and mechanical flexibility.

17. Find the ~~so~~ wavefunction of particle confined in a 1D Box potential or Quantum well.

⟶ Let, consider a particle is confined in a thin sheet of thickness a along the x direction by infinite potential barriers, which create a quantum well as shown in the below figure.



The potential function is –

$$V(x) = 0 \quad \text{for} \quad 0 \le x \le a$$
$$= \infty \quad \text{for otherwise.}$$

The schrodinger equation is -

$$-\frac{\hbar^2}{2m}\cdot\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi$$

For region - II , $V = 0$

$\therefore$ The schrodinger equation will be -

$$-\frac{\hbar^2}{2m}\cdot\frac{\partial^2\psi}{\partial x^2} = E\psi$$

or, $$\frac{\partial^2\psi}{\partial x^2} + \frac{2mE}{\hbar^2}\psi = 0$$

or, $$\frac{\partial^2\psi}{\partial x^2} + K^2\psi = 0 \quad \left[\text{let, } K^2 = \frac{2mE}{\hbar^2}\right]$$

$\longleftarrow$ (i)

The general solution of the equation (i) will be -

$$\psi = A\cos Kx + B\sin Kx$$

Now, for $x = 0$, $\psi = 0$ as $V(x) = \infty$ at $x = 0$.

$\therefore$ $0 = A$ so, $\psi = B\sin Kx$

~~Again at $x = 0$, $\frac{\partial\psi}{\partial x} = 0$ as $V(x) = \infty$ at $x = 0$.~~

Again at $x = a$, $\psi = 0$ as $V(a) = \infty$ at $x = a$.

$\therefore$ $0 = B\sin Ka$

or, $\sin Ka = \sin(n\pi)$ [as $B \neq 0$]

or, $K = \frac{n\pi}{a}$

$\therefore$ $\psi = B\sin\frac{n\pi x}{a}$

Now, using the normalization condition of wavefunction,

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

$$\text{or, } B^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) = 1$$

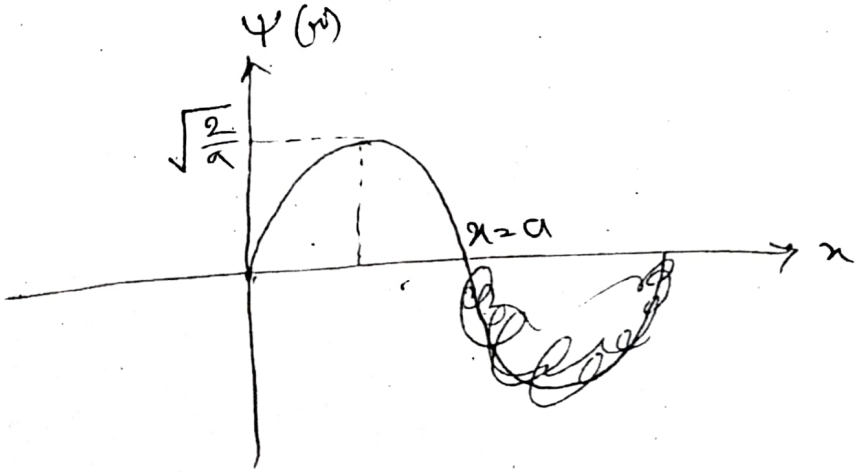
$$\text{or, } \frac{B^2}{2}\left[x - \frac{\sin\left(\frac{2n\pi x}{a}\right)}{\frac{n\pi}{a}}\right]_0^a = 1$$

$$\text{or, } \frac{aB^2}{2} = 1$$

$$\text{or, } B = \sqrt{\frac{2}{a}}$$

$$\therefore \psi = \sqrt{\frac{2}{a}} \cdot \sin\left(\frac{n\pi x}{a}\right)$$

—— This is the wavefunction for a particle confined in a Quantum well.



18. Explain the quantum transport in Quantum dots:

→ Quantum transport in quantum dots refers to the flow electrons through these tiny, nanoscale systems. The unique properties of quantum dots, such as their discrete energy levels and strong electron-electron interactions, lead to various quantum transport phenomena.

In a quantum dot, the electrons occupy specific energy levels, similar to atomic orbitals. This leads to effects like coulomb blockade, where adding each electron requires a specific charging energy. The discrete energy spectrum also allows for observation of quantum interference effects, such as Aharonov-Bohm oscillations in the conductance of quantum dot devices.

The small size of quantum dots means that electron-electrons interactions play a dominant role in determining the transport properties. This cause ~~the~~ the breakdown of the Fermi liquid theory ~~that describ~~ describes electron transport in extended systems.

Quantum dots can be coupled together to form artificial molecules or solids, where the coupling between dots influences the overall transport ~~characteris~~ characteristics. For example, in one-dimensional chains of quantum dots, the disorder in dot sizes can lead to Anderson localization of the electron wavefunc, limiting the conductance.

Thin films :-

A thin film is a layer of materials with thickness ranging from fractions of a nanometer to several micrometers. Thin film may be composed of single layer of atoms or may consists of more than one layer of atoms grown one to other. Thin films are two-D structures in which properties may be dominated by surface and interface effects. If their thickness lies in the quantum size regime, than they may reflect the confinement of electrons in the direction perpendicular to the film.